Macroscopic spin tunneling and quantum critical behavior of a condensate in double-well potential

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In a previous work [1], we have shown that a spinor condensate confined in a periodic or double-well potential exhibits ferromagnetic behavior due to the magnetic dipole-dipole interactions between different wells, and in the absence of external magnetic field, the ground state has a two-fold degeneracy. In this work, we demonstrate the possibility of observing macroscopic quantum spin tunneling between these two degenerate states and show how the tunneling rate critically depends on the strength of the transverse field.

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Tunneling, a process in which a system penetrates into a classically forbidden region (e.g., a potential barrier), is an intrinsically quantum effect with no classical counterpart. Of all tunneling effects, macroscopic quantum tunneling (MQT), the tunneling of a macroscopic variable of a macroscopic system [2], represents a particularly intriguing and interesting scenario as it touches the boundary between the classical and the quantum world and may help shed light on the quantum-classical interface. As such, it is one of the most striking manifestations of quantum mechanics. The tunneling of large magnetic spins has recently received much attention, both theoretically and experimentally [3, 4] in view of its promise as one of the few realistic candidates for an experimental demonstration of MQT, and also because of its connection to quantum computing. Despite considerable efforts, though, there are not many clear and definitive demonstrations of MQT in spin systems so far — although there have been some indications that tunneling might be the underlying reason for some observed results [4, 5]. The reasons for this difficulty are as follows: First, most theories apply to single system, while the conventional magnetic materials used in the experiments contain many domains, each possessing its own set of parameters such as magnetic anisotropy and barrier energy; second, due to the difficulty of cooling the samples down to ultracold temperatures, thermal processes cannot be completely excluded; and third, the spins in solid materials are inevitably imbedded in a crystal matrix and the spin-matrix interaction [6] complicates the physical picture. For these reasons, macroscopic spin tunneling remains one of the most anticipated, yet elusive, quantum phenomena.

In this paper, we demonstrate the possibility of observing spin tunneling in a spinor atomic condensate trapped in a double-well potential, thereby eliminating most of these difficulties. We remark at the outset that while the inter-well tunneling of condensates has been previously considered, all previous studies focused instead on the tunneling of an *external* degree of freedom, the condensate center-of-mass motion [7, 8, 9, 10].

In an earlier paper [1], we showed that because of the long range magnetic dipole-dipole interaction, a spinor atomic condensate trapped in a one-dimensional periodic lattice potential or a double-well potential behaves as a ferromagnet. In the absence of external magnetic fields, the ground state spins of the "mini-condensates" confined in individual wells all align parallel to each other and along the lattice direction (the z-axis), giving rise to a spontaneous magnetization along z. For the sake of simplicity, we restrict the present discussion to a double-well potential, each well containing N spin-1 condensate atoms. In the tight-binding approximation [7], they are described by the zero-temperature spin Hamiltonian [1]

$$H = \lambda'_a(\mathbf{S}_1^2+\mathbf{S}_2^2) - 3\lambda S_1^z S_2^z + \lambda \mathbf{S}_1\cdot\mathbf{S}_2 - h(S_1^x+S_2^x), \quad (1)$$

where $\mathbf{S}_i$ is the total spin of the condensate in the $i^{\rm th}$ well, and $S_i^{x,y,z}$ its cartesian components. The first term in (1) represents the on-site Hamiltonian of the spinor condensate. It includes short-range nonlinear spin-exchange interactions [11], where the parameter λ'_a is related to the s-wave scattering lengths [12] and needs to be negative. The second and third terms in (1) arise from the site-to-site dipole-dipole interaction [1], where $\lambda \equiv \gamma_B^2\mu_0/(4\pi r^3)$ for pure magnetic dipolar interaction, with γ_B being the gyromagnetic ratio, μ_0 the vacuum permeability and r the distance between the two wells. The value of λ can be greatly enhanced by the light-induced optical dipolar interaction if one chooses appropriate laser fields to form the potential well [13, 14]. The last term describes the effect of an external transverse magnetic field, taken to be along the x-axis without the loss of generality. Here $h = \gamma_B B$, with B being the strength of the applied field. In the following, we assume that the nonlinear short-range atom-atom interaction is strong enough that the first term in Hamiltonian (1) dominates over the magnetic dipolar interaction [15]. As a result, the total spin quantum number for each mini-condensate is fixed to its maximum value N — the number of particles in each well. We can therefore neglect the first term in the Hamiltonian (1), since it is a constant of motion and commutes with the remaining terms.

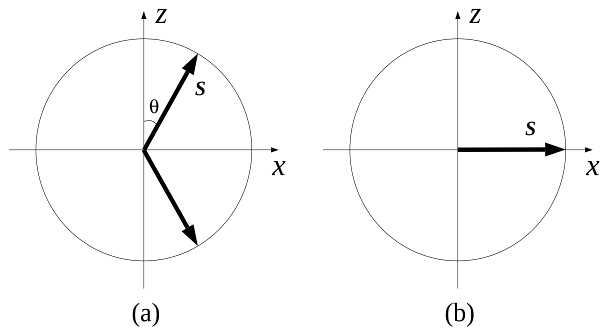

FIG. 1: Classical ground state spin orientation. (a) For $0 \leq h < 3N\lambda$, the ground state has a two-fold degeneracy. (b) For $h > 3N\lambda$, the degeneracy is removed and the spins are polarized along the transverse field.

Before discussing quantum mechanical spin tunneling, let us first investigate the classical situation. The Hamiltonian in that limit is still given by (1), except that the spins are now c-numbers that can be represented by vectors of fixed length N in spin space. For zero field, $h = 0$, it is easy to see that the classical ground state is two-fold degenerate with $\mathbf{S} = \mathbf{S}_1 = \mathbf{S}_2$ pointing along either the z- or $(-z)$-axis. Under the influence of a weak transverse field along the x-direction, the two ground states move away from the z-axis and towards the x-axis while remaining in the xz-plane, as shown in Fig. 1. For $0 \leq h < h_c^{(c)} = 3N\lambda$, the two minima are located at

$$\theta = \pi/2 \pm \cos^{-1}\left(h/h_c^{(c)}\right),$$

where θ is the angle between $\mathbf{S}$ and the z-axis. For $h \geq h_c^{(c)}$, the two minima merge along the x-axis, and the degeneracy is removed. Hence $h_c^{(c)}$ can be regarded as the classical critical field strength, beyond which the system is completely polarized by the external field.

Let us now turn to a quantum mechanical description of the system. Our goal is to investigate whether or not tunneling is present in the classically degenerate regime (i.e., when $0 \leq h < h_c^{(c)}$). We will present both a full numerical calculation and analytical results using the instanton technique.

A well-known consequence of the tunneling between two degenerate states is the lifting of their degeneracy: The two new eigenstates are a symmetric and an anti-symmetric superposition of the original states characterized by an energy difference (or tunneling splitting) $\Delta\varepsilon$ inversely proportional to the tunneling rate. The quantity of interest to determine the occurrence of tunneling is therefore this energy difference between the two lowest eigenstates of the Hamiltonian. We determine it by expanding the Hamiltonian (1) onto the basis spanned by $S_1^z \otimes S_2^z$, and evaluate numerically the eigenvalues of the resultant $(2N+1)^2 \times (2N+1)^2$ matrix. Fig. 2(a) summarizes the result of this analysis. It shows that $\Delta\varepsilon$ is essentially zero for small values of h, but becomes finite when h exceeds a threshold value $h_c^{(q)}$ — the quantum critical field strength. This means that for $0 \leq h \leq h_c^{(q)}$, quantum mechanics agrees with classical mechanics in that the system is degenerate. However, for $h_c^{(q)} < h < h_c^{(c)}$, even though the system is still degenerate in the classical picture, the presence of tunneling removes the degeneracy in the quantum treatment. Fig. 2(b) displays $h_c^{(q)}$ as a function of N, from which one sees that $h_c^{(q)}$ increases with N and approaches $h_c^{(c)}$ as N tends to infinity. In other words, as N increases, the system, as expected, behaves more and more classically.

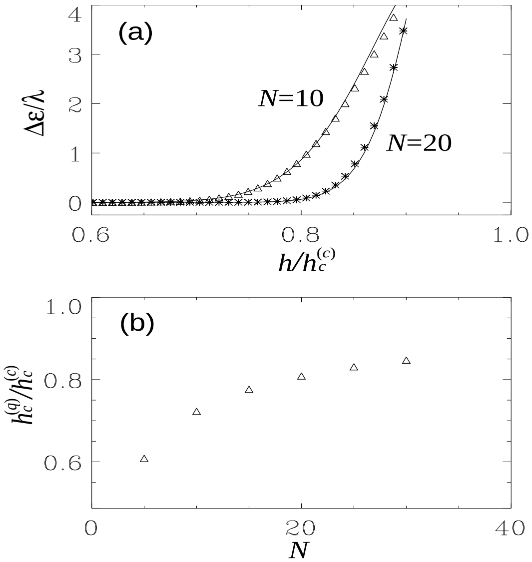

FIG. 2: (a) Energy splitting $\Delta\varepsilon$ as a function of the transverse field strength. The symbols represent numerical results and the solid curves are analytical results obtained from Eq. (3). (b) The quantum critical field strength $h_c^{(q)}$ as a function of N. $h_c^{(q)}$ is defined as the value of h at which $\Delta\varepsilon = 0.1\lambda$.

To gain some analytical insight, we first notice that Hamiltonian (1) can be rewritten as

$$H = -\frac{3\lambda}{4}[(S^z)^2 - (S'^z)^2] + \frac{\lambda}{2}\mathbf{S}^2 - hS^x$$

where $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and $\mathbf{S}' = \mathbf{S}_1 - \mathbf{S}_2$. For $h < h_c^{(c)}$, $\mathbf{S}_1$ and $\mathbf{S}_2$ are tightly bound together, such that $S'^z \approx 0$ and $\mathbf{S}$ is approximately a constant of motion with quantum number $S = 2N$. Hence, neglecting the constant terms, the effective Hamiltonian of the system reads

$$H_{\text{eff}} = -\frac{3\lambda}{4}(S^z)^2 - hS^x. \tag{2}$$

Hamiltonian (2) describes a quantum spin with the easy-axis anisotropy in a transverse field and it has been extensively studied in the context of spin tunneling [3]. Using the instanton technique, which has been proved to

be quite accurate for $S > 5$, the tunneling splitting between the two classically degenerated ground states can be expressed as [16]

$$\Delta\varepsilon = p\omega\sqrt{S_c/(2\pi)}\, e^{-S_c}, \tag{3}$$

where p is a prefactor on the order of unity [by fitting the numerical results with Eq. (3), we find $p \approx 2.75$], $\omega = h_c^{(c)} x$ is the typical instanton frequency with $x = \sqrt{1-(h/h_c^{(c)})^2}$, and $S_c = 2N\ln[(1+x)(1-x)] - 4Nx$ is the classical action. The solid curves in Fig. 2(a) represent the values calculated using Eq. (3), which agree well with the numerical results.

A more intuitive understanding of this threshold behavior in quantum tunneling can be obtained from a quantum perturbation viewpoint. Tunneling results from the transverse magnetic field. If we regard the last term in Hamiltonian (1) as a perturbation to the rest of the Hamiltonian, which possesses two degenerated ground states $|N,N\rangle$ and $|-N,-N\rangle$, where we have labelled the states with the eigenvalues of S_1^z and S_2^z, the tunneling level splitting is then, in the high order perturbation theory [17], given by the shortest chain of matrix elements and energy denominators connecting these two states [18]. For the situation at hand, this chain can be represented as

$$|N,N\rangle \;\Rightarrow\; \frac{1}{\sqrt{2}}(|N-1,N\rangle + |N,N-1\rangle) \Rightarrow |N-1,N-1\rangle \Rightarrow \frac{1}{\sqrt{2}}(|N-2,N-1\rangle + |N-1,N-2\rangle) \Rightarrow$$
$$... \Rightarrow \frac{1}{\sqrt{2}}(|-N,-N+1\rangle + |-N+1,-N\rangle) \Rightarrow |-N,-N\rangle.$$

Since the spin has to travel a distance of $4N$ to reach from one ground state to the other, the tunneling appears minimally in the $(4N)^{\text{th}}$ order of perturbation theory. The energy splitting associated with this chain can be calculated as

$$\begin{aligned}\Delta\varepsilon &= 16\lambda\left(\frac{h}{2\sqrt{2}\lambda}\right)^{4N}\left[\frac{\Gamma\left(3/2+\sqrt{N^2+1/4}-N\right)}{\Gamma\left(N+\sqrt{N^2+1/4}-1/2\right)}\right]^2 \\ &\approx 8\lambda N^2\left(\frac{eh}{4\sqrt{2}N\lambda}\right)^{4N},\end{aligned}$$

where the last line is obtained under the limit $N \ll 1$. The power law dependence on the field strength indicates that $\Delta\varepsilon$ is vanishingly small for large N unless the term inside the bracket exceeds one, resulting in a critical field strength at $(4\sqrt{2}/e)N\lambda \approx 0.7h_c^{(c)}$. Although this treatment explains the threshold behavior, it fails to predict accurately the critical field strength. In particular, it fails to predict the N-dependence of the ratio $h_c^{(q)}/h_c^{(c)}$ [see Fig. 2(b)] . This failure can be easily understood since for h close to the critical point, it is no longer valid to regard the transverse field as a perturbation.

We now turn to the detection of tunneling. It is not practical to directly measure the energy difference between the two lowest energy states, since $\Delta\varepsilon$ is relatively small compared to the total ground state energy. Instead, we use a method which is perfectly suited for the situation at hand, where thermal effects are negligible, but may not be appropriate for more traditional solid-state systems. Our proposed detection scheme starts with the system prepared in one of the degenerated ground state, say, $|N,N\rangle$. The external field h is then slowly ramped up from zero to a final value, $h_f < h_c^{(c)}$. Classically, the macroscopic spin would simply adiabatically follow the instantaneous ground state closest to the initial state. Quantum mechanically, though, this is only true as long as $h_f < h_c^{(q)}$. But for $h_f > h_c^{(q)}$, the system is in the quantum tunneling regime and does not reach an equilibrium. Rather, it oscillates back and forth between the two classically degenerate states, a phenomenon termed as *macroscopic quantum coherence*. The observation of such oscillation will be a direct signature of quantum tunneling, but it requires the effect of dissipation to be small. Otherwise, spin relaxation will result, which is normally the case for the experiment on solid magnetic materials. The long coherence time associated with the atomic condensate, however, makes it ideal for this purpose. In fact, macroscopic center-of-mass oscillation has already been observed in ultracold atoms trapped in optical lattices [9]. Fig. 3 depicts the numerical simulation of the measurement scheme in both the classical and quantum treatments. The quantum mechanical results are obtained by time evolving the Schrödinger equation in spin space with Hamiltonian (1), using the Crank-Nicolson method, while the classical results are obtained by solving the dynamical equation

$$\frac{d\mathbf{S}_i}{dt} = -\gamma_B \mathbf{S}_i \times \frac{\delta H}{\delta \mathbf{S}_i}, \tag{4}$$

where H is the energy functional and has the same form as Hamiltonian (1) but with the spin operators treated as c-numbers. Fig. 3(a) is for $h_f < h_c^{(q)}$. There is no qualitative difference between the quantum and classical

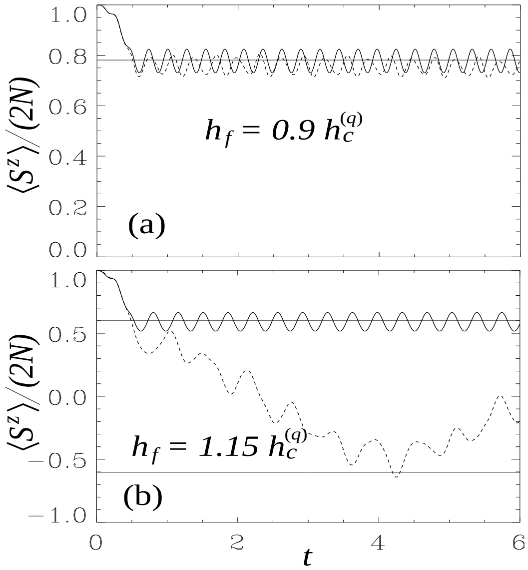

FIG. 3: Time evolution of the expectation value of S^z. Here $N = 10$. The solid lines represent the classical results and the dashed lines the quantum mechanical results. The strength of the transverse field, h, is ramped linearly from 0 to h_f from $t = 0$ to $t = 0.5$, then stays at h_f afterwards. For (a), $h_f = 0.9h_c$, no tunneling is present; for (b), $h_f = 1.15h_c$, macroscopic quantum coherence due to spin tunneling can be observed in the quantum mechanical results. The horizontal lines represent $S^z = \pm 2N\sqrt{1 - [h_f/(3N\lambda)]^2}$, values of S^z in the classical ground state with $h = h_f$. The units for time is $\hbar/\lambda$, which is on the order of a few seconds for typical atomic parameters for pure magnetic dipolar interaction.

results, a steady state is reached in the end (small oscillations around this steady state persists due to nonadiabiticity). Fig. 3(b) is for $h_f > h_c^{(q)}$. The classical result is quite similar to that of Fig. 3(a). However, the quantum calculation clearly shows the oscillations of the system between the two macroscopically distinct states. These two states differ by a minus sign in the expectation value of S^z, which can be easily measured experimentally using, for example, Stern-Gerlach technique [9].

In conclusion, we have shown that the quantum macroscopic tunneling of spin is possible in a spinor condensate trapped in double-well potential. Compared to the more conventional solid state magnetic materials, our system possesses several decisive advantages. First and perhaps foremost, this is an exceedingly clean system characterized by a few simple parameters, without the complication of domain separations, and with well-understood microscopic physics; It is amenable to exquisite experimental control; A single parameter — the transverse field strength — is capable of switching on and off the tunneling. Typical temperatures of the atomic condensate is in the nanoKelvin regime, hence the thermal activation normally presented in the solid materials can be safely neglected [19]. Due to these reasons, we believe that this system is indeed ideal for studying quantum magnetism in general [1, 13], and macrosopic quantum tunneling in particular. Finally we remark that although we have considered a double-well potential in this work, we expect similar behavior for a condensate confined in a one-dimensional periodic lattice potential.

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